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## **Report Title**

Materials on the brink: unprecedented transforming materials.

### **ABSTRACT**

This report documents the progress of the MURI on 'Materials on the brink: Unprecedented transforming materials' for the period of 2012-2013.

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**Enter List of papers submitted or published that acknowledge ARO support from the start of the project to the date of this printing. List the papers, including journal references, in the following categories:**

**(a) Papers published in peer-reviewed journals (N/A for none)**

- 02/06/2013    49.00   JiangYu Li. On the depolarization Energy of Ferroelectrics, Mechanics of Materials, (10 2009): 1125. doi:
- 02/06/2013    84.00   Daisuke Kan, Richard Suchoski, Shigehiro Fujino, Ichiro Takeuchi. COMBINATORIAL INVESTIGATION OF STRUCTURAL AND FERROELECTRIC PROPERTIES OF A- AND B-SITE CO-DOPED BiFeO<sub>3</sub> THIN FILMS, Integrated Ferroelectrics,, (03 2010): 116. doi:
- 02/06/2013    83.00   Ø. Prytz, A.E. Gunnæs, O.B. Karlsen, T.H. Breivik, E.S. Toberer, G. Jeffrey Snyder, J. Taftø. Nanoscale inclusions in the phonoglass thermoelectric material Zn<sub>4</sub>Sb<sub>3</sub>, Philosophical Magazine Letters, (06 2009): 362. doi:
- 02/06/2013    81.00   Eric S. Toberer, Teruyuki Ikeda, Vilupanur A. Ravi, G. Jeffrey Snyder, hinobu Aoyagi, Eiji Nishibori , Makoto Sakata. In situ observation of eutectoid reaction forming a PbTe-Sb<sub>2</sub>Te<sub>3</sub> thermoelectric nanocomposite by synchrotron X-ray diffraction, Scripta Materialia, (03 2009): 321. doi:
- 02/06/2013    82.00   Teruyuki Ikeda, Vilupanur A. Ravi, G. Jeffrey Snyder. Evaluation of true inter-lamellar spacing from microstructural observations , Journal of Materials Research, (01 2008): 2538. doi:
- 02/06/2013    80.00   Teruyuki Ikeda, Vilupanur A. Ravib , G. Jeffrey Snyder. Formation of Sb<sub>2</sub>Te<sub>3</sub> Widmanstätten precipitates in thermoelectric PbTe, Acta Materialia, (02 2009): 666. doi:
- 02/06/2013    79.00   Matthew J. Dicken, Koray Aydin , Imogen M. Pryce, Luke A. Sweatlock , Elizabeth M. Boyd , Sameer Walavalkar , James Ma , Harry A. Atwater . Frequency tunable near-infrared metamaterials based on VO<sub>2</sub> phase transition, Optics Express, (09 2009): 18330. doi:
- 02/06/2013    78.00   Y. Y. Liu , J. Y. Li. Energetic analysis of ferroelectric domain patterns by equivalent inclusion method, Journal of Materials Science, (05 2009): 5214. doi:
- 02/06/2013    77.00   Mark Laver, Shenqiang Ren, Manfred Wuttig. Nanolamellar magnetoelectric BaTiO<sub>3</sub>-CoFe<sub>2</sub>O<sub>4</sub> bicrystal , Applied Physics Letters (accepted), (10 2009): 153504. doi:
- 02/06/2013    74.00   Richard D. James, Stefan Müller, Zhiyong Zhang. Energy barriers and hysteresis in martensitic phase transformations, Acta Materialia, (09 2009): 4332. doi:
- 02/06/2013    76.00   Rémi Delville, Dominique Schryvers, Zhiyong Zhang, Richard D. James. Transmission electron microscopy investigation of microstructures in low-hysteresis alloys with special lattice parameters, Scripta Materialia, (03 2009): 293. doi:
- 02/06/2013    67.00   M. Murakami, S.-H. Lim, J. H. Yang, S.-Y. Young, J. Hattrick-Simpers, M. Wuttig, L. G. Salamanca-Riba, I. Takeuchi. Enhanced dielectric properties in single crystal-like BiFeO<sub>3</sub> thin films grown by flux-mediated epitaxy , Applied Physics Letters, (01 2008): 12918. doi:
- 02/06/2013    73.00   W. Tanga, D.N. Fanga, J.Y. Lib. Two-scale micromechanics-based probabilistic modeling of domain switching in ferroelectric ceramics, Journal of the Mechanics and Physics of Solids, (10 2009): 1683. doi:
- 02/06/2013    75.00   Rémi Delville , Sakthivel Kasinathan, Zhiyong Zhang, Jan Van Humbeeck , Richard D. James, Dominique Schryvers. Transmission electron microscopy study of phase compatibility in low hysteresis shape memory alloys, Philosophical Magazine, (01 2010): 177. doi:

- 02/06/2013 72.00 Shenqiang Ren, Robert M. Briber, Manfred Wuttig. Self-organized two-dimensional onions, *Applied Physics Letters*, (03 2009): 113507. doi:
- 02/06/2013 71.00 N. D. Orloff, W. Tian, C. J. Fennie, C. H. Lee, D. Gu, J. Mateu, X. X. Xi, K. M. Rabe, D. G. Schlom, I. Takeuchi, J. C. Booth. Broadband dielectric spectroscopy of Ruddlesden–Popper  $\text{Sr}_{n+1}\text{Ti}_n\text{O}_{3n+1}$  ( $n = 1,2,3$ ) thin films , *Applied Physics Letters*, (01 2009): 42908. doi:
- 02/06/2013 70.00 S.-H. Lima, M. Murakami, S.E. Lofland, A.J. Zambano, L.G. Salamanca-Riba, I. Takeuchi. Exchange bias in thin-film  $(\text{Co/Pt})_3/\text{Cr}_2\text{O}_3$  multilayers, *Journal of Magnetism and Magnetic Materials*, (07 2009): 1955. doi:
- 02/06/2013 69.00 Ching Jung Cheng, Sung Hwan Lim , Varatharajan Anbusathaiah, Makoto Murakami, Lourdes G. Salamanca-Riba, Ichiro Takeuchi, Valanoor Nagarajan. Role of oxygen partial pressure and seed layer chemistry in flux mediated epitaxy of single phase multiferroic  $\text{BiFeO}_3$  thin films , *Applied Physics Letters*, (11 2008): 192906. doi:
- 02/06/2013 68.00 Yaniv Ganor, Doron Shilo, Thomas W. Shield, Richard D. James. Breaching the work output limitation of ferromagnetic shape memory alloys , *Applied Physics Letters*, (09 2008): 122509. doi:
- 02/06/2013 65.00 Shenqiang Ren, Robert M. Briber, Manfred Wuttig . Diblock copolymer based self-assembled nanomagnetolectric , *Applied Physics Letters*, (10 2008): 173507. doi:
- 02/06/2013 66.00 S. Fujino, M. Murakami, V. Anbusathaiah, S.-H. Lim, V. Nagarajan, C. J. Fennie, M. Wuttig, L. Salamanca-Riba, I. Takeuchi. Combinatorial discovery of a lead-free morphotropic phase boundary in a thin-film piezoelectric perovskite, *Applied Physics Letters* (accepted), (05 2008): 202904. doi:
- 02/06/2013 64.00 L. J. Li, Y. C. Shu, J. H. Yen, J. Y. Li. The magnetoelectric domains and cross-field switching in multiferroic  $\text{BiFeO}_3$ , *Applied Physics Letters*, (11 2008): 192506. doi:
- 02/06/2013 63.00 J. Y. Li, T. Chen. The exact connections of the effective thermal properties of ferroelectric crystals with domain configurations , *Journal of Applied Physics*, (06 2008): 124102. doi:
- 02/06/2013 62.00 L. J. Li, J. Y. Li, Y. C. Shu, H. Z. Chen, J. H. Yen. Magnetoelastic domains and magnetic field-induced strains in ferromagnetic shape memory alloys by phase-field simulation, *Applied Physics Letters*, (04 2008): 172504. doi:
- 02/06/2013 61.00 Shenqiang Ren, Manfred Wuttig. Magnetolectric nano- $\text{Fe}_3\text{O}_4/\text{CoFe}_2\text{O}_4||\text{PbZr}_{0.53}\text{Ti}_{0.47}\text{O}_3$  composite , *Applied Physics Letters*, (02 2008): 83502. doi:
- 02/06/2013 60.00 J.Y. Li, Y.F. Ma. Magnetoelastic modeling of magnetization rotation and variant rearrangement in ferromagnetic shape memory alloys, *Mechanics of Materials*, (12 2008): 1022. doi:
- 02/06/2013 59.00 L. Hong , A. K. Soh, Q. G. Du , J. Y. Li. Interaction of O vacancies and domain structures in single crystal  $\text{BaTiO}_3$ : Two-dimensional ferroelectric model, *Physical Review B*, (03 2008): 94104. doi:
- 02/06/2013 57.00 S.H. Xie, L.P. Tang, X.J. Zheng, Y.C. Zhou, J.Y. Li. Domain switching in ferroelectric ceramics beyond Taylor bound, *Mechanism and Machine Theory*, (04 2007): 362. doi:
- 02/06/2013 58.00 J. H. Yen, Y. C. Shu, H. Z. Chen, J. Y. Li, L. J. Li. Constrained Modeling of Domain Patterns in Rhombohedral Ferroelectrics, *Applied Physics Letters*, (02 2008): 52909. doi:

- 02/06/2013 56.00 Shenqiang Ren\, Manfred Wuttig. Spinodal synthesis of PZT/NFO magnetoelectric, Applied Physics Letters, (08 2007): 83501. doi:
- 02/06/2013 55.00 Y. Y. Liu, J. J. Liu, S. H. Xie, J. Y. Li. Energetics of charged domain walls in ferroelectric crystals, Applied Physics Letters (accepted), (10 2007): 172910. doi:
- 02/06/2013 54.00 M. Murakami, S. Fujino, S.-H. Lim, L. G. Salamanca-Riba, M. Wuttig, I. Takeuchi, Bindhu Varughese, H. Sugaya, T. Hasegawa, S. E. Lofland. Microstructure and phase control in Bi-Fe-O multiferroic nanocomposite thin films , Applied Physics Letters, (03 2006): 112505. doi:
- 02/06/2013 53.00 S.-H. Lima, M. Murakamia, S.E. Loflandb, A.J. Zambanoa, L.G. Salamanca-Riba, I. Takeuchia. Exchange bias in thin-film (Co/Pt)3/Cr2O3 multilayers, Journal of Magnetism and Magnetic Materials, (07 2009): 1955. doi:
- 02/06/2013 52.00 Daisuke Kan, Fransiska C. Kartawidjaja, Reza Mahjoub, Miryam A. Arredondo, Samantha Wicks, Ichiro Takeuchi, John Wang, Valanoor Nagarajan, Varatharajan Anbusathaiah. Labile Ferroelastic Nanodomains in Bilayered Ferroelectric Thin Films, Advanced Materials, (09 2009): 3497. doi:
- 02/06/2013 51.00 Peng Zhao, Zhenli Zhao, Dwight Hunter, Richard Suchoski, Chen Gao, Scott Mathews, Manfred Wuttig, Ichiro Takeuchi<sup>1</sup>. Fabrication and characterization of all-thin-film magnetoelectric sensors, Applied Physics Letters, (06 2009): 243507. doi:
- 02/06/2013 50.00 C.-J. Cheng, D. Kan, S.-H. Lim, W. R. McKenzie, P. R. Munroe, L. G. Salamanca-Riba, R. L. Withers, I. Takeuchi, V. Nagarajan. Structural transitions and complex domain structures across a ferroelectric-to-antiferroelectric phase boundary in epitaxial Sm-doped BiFeO<sub>3</sub> thin films, Physical Review B (accepted), (07 2009): 1409. doi:
- 02/27/2013 89.00 L. J. Li, Y. C. Shu, C. H. Lei, J. Y. Li. Austenite-martensite interface in shape memory alloys, Applied Physics Letters, (04 2010): 141910. doi:
- 02/27/2013 06.00 Vijay Srivastava, Xian Chen, Richard D. James . Hysteresis and unusual magnetic properties in the singular Heusler alloy Ni<sub>45</sub>Co<sub>5</sub>Mn<sub>40</sub>Sn<sub>10</sub> , Applied Physics Letters (accepted), (07 2010): 14101. doi:
- 02/27/2013 05.00 Ching-Jung Cheng, Daisuke Kan, Varatharajan Anbusathaiah, Ichiro Takeuchi, Valanoor Nagarajan. Microstructure-electromechanical property correlations in rare-earth substituted BiFeO<sub>3</sub> epitaxial thin films at morphotropic phase boundaries , Applied Physics Letters, (11 2010): 212905. doi:
- 02/27/2013 04.00 Todd Brintlinger, Sung-Hwan Lim, Kamal H. Baloch, Paris Alexander, Yi Qi, John Barry, John Melngailis , Lourdes Salamanca-Riba, I. Takeuchi, John Cumings. In Situ Observation of Reversible Nanomagnetic Switching Induced by Electric Fields , Nano Letters, (03 2010): 1219. doi:
- 02/27/2013 03.00 Ching-Jung Cheng , Albina Y. Borisevich, Daisuke Kan , Ichiro Takeuchi, Valanoor Nagarajan. Nanoscale Structural and Chemical Properties of Antipolar Clusters in Sm-Doped BiFeO<sub>3</sub> Ferroelectric Epitaxial Thin Films , Chemistry of Materials, (02 2010): 2588. doi:
- 02/27/2013 02.00 Daisuke Kan, Lucia Pálová, Varatharajan Anbusathaiah, Ching Jung Cheng, Shigehiro Fujino, Valanoor Nagarajan, Karin M. Rabe, Ichiro Takeuchi. Universal Behavior and Electric-Field-Induced Structural Transition in Rare-Earth-Substituted BiFeO<sub>3</sub>, Advaced Functional materials , (04 2010): 1108. doi:
- 02/27/2013 01.00 Robert Zarnetta, Ryota Takahashi, Marcus L. Young, Alan Savan, Yasubumi Furuya, Sigurd Thienhaus, Burkhard Maa, Mustafa Rahim, Jan Frenzel, Hayo Brunken, Yong S. Chu, Vijay Srivastava, Richard D. James, Ichiro Takeuchi, Gunther Eggeler, Alfred Ludwig. Identification of quaternary shape memory alloys with near zero thermal hysteresis and unprecedented functional stability, Advaced Functional materials , (06 2010): 1917. doi:

- 02/27/2013 00.00 Daisuke Kan, Ichiro Takeuchi . Effect of substrate orientation on lattice relaxation of epitaxial BiFeO<sub>3</sub> thin films ,  
Journal of Applied Physics, (07 2010): 14104. doi:
- 02/27/2013 99.00 S. B. Emery,, C.-J. Cheng,, D. Kan, F. J. Rueckert, S. P. Alpay, V. Nagarajan, I. Takeuchi, B. O. Wells. Phase coexistence near a morphotropic phase boundary in Sm-doped BiFeO<sub>3</sub> films,  
Applied Physics Letters, (10 2010): 152902. doi:
- 02/27/2013 98.00 Jonghee Lee, Christian J. Long, Haitao Yang, Xiao-Dong Xiang, Ichiro Takeuchi1 . Atomic resolution imaging at 2.5 GHz using near-field microwave Microscopy ,  
Applied Physics Letters, (11 2010): 183111. doi:
- 02/27/2013 97.00 Teruyuki Ikeda, Vilupanur A. Ravi, G. Jeffrey Snyder . Microstructure Size Control through Cooling Rate in Thermoelectric PbTe-Sb<sub>2</sub>Te<sub>3</sub> Composites ,  
Metallurgical and Materials Transactions A , (03 2010): 641. doi:
- 02/27/2013 96.00 Teruyuki Ikeda, G. Jeffrey Snyder, Chris Dames, Fan Yang. Effective thermal conductivity of polycrystalline materials with randomly oriented superlattice grains ,  
Journal of Applied Physics, (08 2010): 34310. doi:
- 02/27/2013 94.00 U.K. Roessler, O. Heczko, M. Wuttig, J. Buschbeck, S. Kaufmann, L. Schultz, S. Fahler. Adaptive modulations of martensites ,  
Physical Review Letters (accepted), (04 2010): 145702. doi:
- 02/27/2013 93.00 Antje Dannenberg, Mario Siewert, Markus E. Gruner, Manfred Wuttig, Peter Entel. Competing structural ordering tendencies in Heusler-type alloys with high Curie ,  
Phys. Rev. B , (12 2010): 214421. doi:
- 02/27/2013 95.00 M. Laver, Mudivarathi, J. R. Cullen, A. B. Flatau, W.-C. Chen, S. M. Watson, M. Wuttig. Magnetostriction and Magnetic Heterogeneities in Iron-Gallium,  
Physical Review Letters (accepted), (07 2010): 27202. doi:
- 02/27/2013 91.00 Y.Y. Liu, Z.X. Zhu, J.-F. Li, J.Y. Li . Misfit strain modulated phase structures of epitaxial Pb(Zr<sub>1-x</sub>Ti<sub>x</sub>)O<sub>3</sub> thin films: The effect of substrate and film thickness,  
Mechanics of Materials, (08 2010): 816. doi:
- 02/27/2013 92.00 S. H. Xie, Y. M. Liu, X. Y. Liu, Q. F. Zhou, K. K. Shung, Y. C. Zhou, J. Y. Li. Local two-way magnetoelectric couplings in multiferroic composites via scanning probe microscopy ,  
Journal of Applied Physics, (09 2010): 54108. doi:
- 02/27/2013 90.00 D. N. Fang, W. Tang, J. Y. Li . Spinodally synthesized magnetoelectric,  
Ferroelectrics, (01 2010): 196. doi:
- 02/27/2013 88.00 Y. Y. Liu, J. Y. Li. Space charges and size effects in semiconducting ferroelectric BaTiO<sub>3</sub>/SrTiO<sub>3</sub> superlattices,  
Applied Physics Letters, (07 2010): 42905. doi: 10.1063/1.3473821
- 02/27/2013 87.00 L.J. Li, Y. Yang , Y.C. Shu , J.Y. Li. Continuum theory and phase-field simulation of magnetoelectric effects in multiferroic bismuth ferrite,  
Journal of the Mechanics and Physics of Solids, (10 2010): 1613. doi:
- 02/27/2013 86.00 Ayako Ikeda , Sossina M. Haile. Examination of the superprotonic transition and dehydration behavior of Cs<sub>0.75</sub>Rb<sub>0.25</sub>H<sub>2</sub>PO<sub>4</sub> by thermogravimetric and differential thermal analyses,  
Solid State Ionics, (01 2010): 193. doi:
- 02/27/2013 85.00 Mikhail Kislitsyn, Mary W. Louie , Kaushik Bhattacharya, Sossina M. Haile. Phase transformation and hysteresis behavior in Cs<sub>1-x</sub>Rb<sub>x</sub>H<sub>2</sub>PO<sub>4</sub>,  
Solid State Ionics, (01 2010): 173. doi:
- 08/30/2013 26.00 Phanish Suryanarayana, Kaushik Bhattacharya. Evolution of polarization profiles and switching in ferroelectric thin films.,  
Journal of Applied Physics, (02 2012): 34109. doi:

- 08/30/2013 25.00 Richard D. James. Enhanced reversibility and unusual microstructure of a phase-transforming material, *Nature*, (02 2013): 0. doi:
- 08/30/2013 23.00 Yintao Song, Kanwal Preet Bhatti, Vijay Srivastava, C. Leighton, Richard D. James. Thermodynamics of energy conversion via first order phase transformation in low hysteresis magnetic materials, *Energy & Environmental Science*, (02 2013): 1315. doi: 10.1039/c3ee24021e
- 08/30/2013 22.00 S. El-Khatib, Vijay Srivastava, R. D. James, C. Leighton, Kanwal Preet Bhatti. Small-angle neutron scattering study of magnetic ordering and inhomogeneity across the martensitic phase transformation in  $\text{Ni}_{50-x}\text{Co}_x\text{Mn}_{40}\text{Sn}_{10}$  alloys, *Physical Review B*, (04 2012): 134450. doi: 10.1103/PhysRevB.85.134450
- 08/30/2013 21.00 M. B. Okatan, R. K. Vasudevan, Y. Y. Liu, S. Jesse, J.-C. Yang, W.-I. Liang, Y.-H. Chu, J. Y. Li, S. V. Kalinin, V. Nagarajan. Unraveling the origins of electromechanical response in mixed-phase bismuth ferrite, *Physical Review B*, (07 2013): 20402. doi: 10.1103/PhysRevB.88.020402
- 08/30/2013 15.00 Yoshiki Takagiwa, Yanzhong Pei, Gregory Pomrehn, G. Jeffrey Snyder. Validity of rigid band approximation of PbTe thermoelectric materials, *Applied Physics Letters Materials*, (06 2013): 11101. doi: 10.1063/1.4809545
- 08/30/2013 14.00 Alex Zevalkink, Wolfgang G. Zeier, Gregory Pomrehn, Eugen Schechtel, Wolfgang Tremel, G. Jeffrey Snyder. Thermoelectric properties of  $\text{Sr}_3\text{GaSb}_3$  – a chain-forming Zintl compound, *Energy & Environmental Science*, (09 2012): 9121. doi: 10.1039/c2ee22378c
- 08/30/2013 13.00 Alex Zevalkink, Jessica Swallow, G. Jeffrey Snyder. Thermoelectric properties of Zn-doped  $\text{Ca}_5\text{In}_2\text{Sb}_6$ , *Dalton Transactions*, (07 2013): 9713. doi: 10.1039/c3dt50428j
- 08/30/2013 12.00 Wolfgang G. Zeier, Yanzhong Pei, Gregory Pomrehn, Tristan Day, Nicholas Heinz, Christophe P. Heinrich, G. Jeffrey Snyder, Wolfgang Tremel. Phonon Scattering through a Local Anisotropic Structural Disorder in the Thermoelectric Solid Solution Cu, *Journal of the American Chemical Society*, (01 2013): 726. doi: 10.1021/ja308627v
- 08/30/2013 11.00 Alex Zevalkink, Gregory S. Pomrehn, Samantha Johnson, Jessica Swallow, Zachary M. Gibbs, G. Jeffrey Snyder. Influence of the Tria Elements ( $M = \text{Al}, \text{Ga}, \text{In}$ ) on the Transport Properties of  $\text{Ca}_5\text{M}_2\text{Sb}_6$  Zintl Compounds, *Chemistry of Materials*, (06 2012): 2091. doi: 10.1021/cm300520w
- 08/30/2013 10.00 Chan-Ho Yang, Daisuke Kan, Ichiro Takeuchi, Valanoor Nagarajan, Jan Seidel. Doping  $\text{BiFeO}_3$ : approaches and enhanced functionality, *Physical Chemistry Chemical Physics*, (10 2012): 15953. doi: 10.1039/c2cp43082g
- 08/30/2013 09.00 Y. Takagiwa, Y. Pei, G. Pomrehn, G. J. Snyder. Dopants effect on the band structure of PbTe thermoelectric material, *Applied Physics Letters*, (08 2012): 92102. doi: 10.1063/1.4748363
- 08/30/2013 08.00 Daisuke Kan, Christian J. Long, Christian Steinmetz, Samuel E. Lofland, Ichiro Takeuchi. Combinatorial search of structural transitions: Systematic investigation of morphotropic phase boundaries in chemically substituted  $\text{BiFeO}_3$ , *Journal of Materials Research*, (09 2012): 2691. doi: 10.1557/jmr.2012.314
- 08/30/2013 07.00 Ichiro Takeuchi, Jason R. Hattrick-Simpers, Martin L. Green. Applications of high throughput (combinatorial) methodologies to electronic, magnetic, optical, and energy-related materials, *Journal of Applied Physics*, (06 2013): 231101. doi: 10.1063/1.4803530
- 08/30/2013 27.00 Vivek B. Shenoy, Yu Xiao, Kaushik Bhattacharya. Effect of doping on polarization profiles and switching in semiconducting ferroelectric thin films, *Journal of Applied Physics*, (04 2012): 0. doi: 10.1063/1.3702849
- 09/06/2013 29.00 Hsin-Yi Kuo, Kaushik Bhattacharya. Fibrous composites of piezoelectric and piezomagnetic phases, *Mechanics of Materials*, (07 2013): 159. doi:

- 09/09/2013 30.00 William Ratcliff II, Daisuke Kan, Wangchun Chen, Shannon Watson, Songxue Chi, Ross Erwin, Garry J. McIntyre, Sylvia C. Capelli, Ichiro Takeuchi. Neutron diffraction investigations of magnetism in BiFeO<sub>3</sub> Epitaxial Films, *Advanced Functional Materials*, (05 2011): 1567. doi:
- 09/10/2013 32.00 Teruyuki Ikeda, Shiho Iwanaga, Hsin-jay Wu, Nathan J. Marolf, Sinn-wen Chen, G. Jeffrey Snyder. A combinatorial approach to microstructure and thermopower of bulk thermoelectric materials: the pseudo-ternary PbTe–Ag<sub>2</sub>Te–Sb<sub>2</sub>Te<sub>3</sub> system, *Journal of Materials Chemistry*, (06 2012): 24335. doi:
- 09/10/2013 31.00 Kristin Bergum, Teruyuki Ikeda, G. Jeffrey Snyder. Solubility and microstructure in the pseudo-binary PbTe–Ag<sub>2</sub>Te system, *Journal of Solid State Chemistry*, (09 2011): 2543. doi:
- 09/10/2013 33.00 Teruyuki Ikeda, Nathan J. Marolf, Kristin Bergum, Marcus B. Toussaint, Nicholas A. Heinz, Vilupanur A. Ravi, G. Jeffrey Snyder. Size control of Sb<sub>2</sub>Te<sub>3</sub> Widmanstätten precipitates in thermoelectric PbTe, *Acta Materialia*, (03 2011): 2679. doi:
- 09/10/2013 34.00 Xian Chena, Vijay Srivastava, Vivekanand Dabade, Richard D. James. Study of the cofactor conditions: Conditions of supercompatibility between phases, *Journal of the Mechanics and Physics of Solids*, (08 2013): 0. doi:
- 12/12/2012 2.00 38. C.T. Nelson, P. Cao, J.R. Jokisaari, C. Heikes, C. Adamo, A. Melville, S.H. Baek, C.M. Folkman, B. Winchester, Y.J. Gu, Y.M. Liu, K. Zhang, E.G. Wang, J.Y. Li, L.Q. Chen, C.B. Eom, D.G. Schlom, and X.Q. Pan. Domain dynamics during ferroelectric switching, *Science*, (11 2011): 968. doi:
- 12/18/2012 3.00 Rama K. Vasudevan, Yunya Liu, Jiangyu Li, Wen-I. Liang, Amit Kumar, Stephen Jesse, Yi-Chun Chen, Ying-Hao Chu, Valanoor Nagarajan, Sergei V. Kalinin. Nanoscale control of phase variants in strain-engineered BiFeO<sub>3</sub>, *Nano Letters*, (06 2011): 3346. doi:
- 12/18/2012 21.00 Nathan J. Marolf, G. Jeffrey Snyder, Teruyuki Ikeda. Zone leveling crystal growth of thermoelectric PbTe alloys with Sb<sub>2</sub>Te<sub>3</sub> Widmanstätten precipitates, *Crystal Growth & Design*, (08 2011): 4183. doi:
- 12/18/2012 20.00 Xian Chena, Shanshan Caob, Teruyuki Ikeda, Vijay Srivastava, G. Jeffrey Snyder, Dominique Schryvers, Richard D. James. A weak compatibility condition for precipitation with application to the microstructure of PbTe–Sb<sub>2</sub>Te<sub>3</sub> thermoelectrics, *Acta Materialia*, (09 2011): 6124. doi:
- 12/18/2012 19.00 Teruyuki Ikeda, Marcus B. Toussaint, Kristin Bergum, Shiho Iwanaga, G. Jeffrey Snyder. Solubility and formation of ternary Widmanstätten precipitates in PbTe in the pseudo-binary, *Journal of Materials Science*, (02 2011): 3846. doi:
- 12/18/2012 18.00 N.A. Heinz, T. Ikeda, G.J. Snyder, D.L. Medlin. Interfacial Disconnections at Sb<sub>2</sub>Te<sub>3</sub> Precipitates in PbTe: Mechanisms of Strain, *Acta Materialia*, (12 2011): 7724. doi:
- 12/18/2012 14.00 Nicholas A. Heinz, Teruyuki Ikeda, G. Jeffrey Snyder. Formation of highly oriented large nanoscale In<sub>2</sub>Te<sub>3</sub> precipitates in bulk Bi<sub>2</sub>Te<sub>3</sub>, *Acta Materialia*, (06 2012): 4461. doi:
- 12/18/2012 13.00 H.-J. Wu, S.-W. Chena, T. Ikeda, G.J. Snyder. Formation of ordered nano-wire microstructures in thermoelectric Pb–Ag–Sb–Te, *Acta Materialia*, (02 2012): 1129. doi:
- 12/18/2012 12.00 Wei-Feng Rao, Manfred Wuttig, Armen G. Khachaturyan. Giant nonhysteretic responses of two-phase nanostructured alloys, *Phys. Rev. Lett.* (submitted), (03 2011): 105703. doi:



- 12/18/2012 11.00 Dwight Hunter, Will Osborn, Ke Wang, Nataliya Kazantseva, Jason Hattrick-Simpers, Richard Suchoski, Ryota Takahashi, Marcus L. Young, Apurva Mehta, Leonid A. Bendersky, Sam E. Lofland, Manfred Wuttig, Ichiro Takeuchi<sup>1</sup>. Giant magnetostriction in annealed Co<sub>1-x</sub>Fe<sub>x</sub> thin-films, Nature Communications, (11 2011): 1. doi:
- 12/18/2012 10.00 M. Siewert, M. E. Gruner, A. Dannenberg, A. Chakrabarti, H. C. Herper<sup>1</sup>, M. Wuttig, S. R. Barman, S. Singh, A. Al-Zubi, T. Hickel, J. Neugebauer, M. Gillessen, R. Dronskowski, P. Entel. Designing shape-memory Heusler alloys from first-principles, Appl. Phys. Lett., (11 2011): 191904. doi:
- 12/18/2012 9.00 Yuanming Liu, Yanhang Zhang, Ming-Jay Chow, Qian Nataly Chen, Jiangyu Li<sup>1</sup>. Biological ferroelectricity uncovered in aortic walls by piezoresponse force microscopy, Phys. Rev. Lett. (submitted), (02 2012): 78103. doi:
- 12/18/2012 8.00 Yuanming Liu, Shuhong Xie, Xiaoyan Liu, Kenji Kitamura, Jiangyu Li. Thermal variation of piezoresponse in microscopically poled poly (vinylidene fluoride-trifluoroethylene) ferroelectric copolymers approaching Curie temperature, J. Appl. Phys., (09 2011): 52008. doi:
- 12/18/2012 7.00 Y. Yang, L. J. Li, J. Y. Li. Monte Carlo simulation of magnetoelectric coupling in multiferroic BiFeO<sub>3</sub>, Appl. Phys. Lett., (05 2011): 182905. doi:
- 12/18/2012 6.00 S. H. Xie, X. Y. Liu, Y. C. Zhou, J. Y. Li<sup>2</sup>. Correlation of magnetic domains and magnetostrictive strains in Terfenol-D via magnetic force microscopy, Journal of Applied Physics (accepted for publication), (03 2011): 63911. doi:
- 12/18/2012 5.00 Shuhong Xie, Feiyue Ma, Yuanming Liu, Jiangyu Li. Multiferroic CoFe<sub>2</sub>O<sub>4</sub>-Pb(Zr<sub>0.52</sub>Ti<sub>0.48</sub>)O<sub>3</sub> core-shell nanofibers and their magnetoelectric Coupling, Nanoscale, (06 2011): 3152. doi:
- 12/18/2012 4.00 Y. Y. Liu, J. Y. Li. Shear-driven morphotropic phase boundary in epitaxial ferroelectric thin films, Phys. Rev. B (submitted), (10 2011): 132104. doi:
- 12/19/2012 36.00 Kanwal Preet Bhatti, S. El-Khatib, Vijay Srivastava, R. D. James, C. Leighton. Small-angle neutron scattering study of magnetic ordering and inhomogeneity across the martensitic phase transformation in Ni<sub>50-x</sub>CoxMn<sub>40</sub>Sn<sub>10</sub> alloys, Physical Review B, (04 2012): 134450. doi:
- 12/19/2012 39.00 Sossina M. Haile, Chatr Panithipongwuta. High-Temperature Phase Behavior in the Rb<sub>3</sub>H(SO<sub>4</sub>)<sub>2</sub>-RbHSO<sub>4</sub> Pseudo-Binary System and the New Compound Rb<sub>5</sub>H<sub>3</sub>(SO<sub>4</sub>)<sub>4</sub>, Solid State Ionics, (04 2012): 53. doi:
- 12/19/2012 38.00 Ayako Ikeda<sup>a</sup>, Sossina M. Haile<sup>a</sup>. The thermodynamics and kinetics of the dehydration of CsH<sub>2</sub>PO<sub>4</sub> studied in the presence of SiO<sub>2</sub>, Solid State Ionics, (04 2012): 63. doi:
- 12/19/2012 37.00 J. Buschbeck, J. Kawasaki, T. E. Buehl, A. C. Gossard, C. J. Palmstrøm. Growth of Epitaxial NiTi Shape Memory Alloy Films on GaAs (001) and Evidence of Martensitic Transformation, Journal of Vacuum Science & Technology B: Microelectronics and Nanometer Structures, (03 2011): 116. doi:
- 12/19/2012 32.00 isuke Kan<sup>1</sup>, Ching-Jung Cheng, Valanoor Nagarajan, Ichiro Takeuchi. Composition and temperature-induced structural evolution in La, Sm, and Dy substituted BiFeO<sub>3</sub> epitaxial thin films at morphotropic phase boundaries, Journal of Applied Physics, (07 2011): 14106. doi:
- 12/19/2012 30.00 Yi Wang, Christian J. Long, Ichiro Takeuchi<sup>1</sup>, Tiberiu-Dan Onuta. Energy harvesting properties of all-thin-film multiferroic cantilevers, Applied Physics Letters, (11 2011): 203506. doi:
- 12/19/2012 29.00 K. Rajan, K. Stoewe, I. Takeuchi, B. Chisholm, H. Lam, R. Potyrailo. Combinatorial and High-Throughput Screening of Materials Libraries: Review of State of the Art, ACS Combinatorial Science, (06 2011): 79. doi:

- 12/19/2012 28.00 Daisuke Kan<sup>†</sup>, Varatharajan Anbusathaiah, Ichiro Takeuchi. Chemical Substitution-Induced Ferroelectric Polarization Rotation in BiFeO<sub>3</sub>, *Advanced Materials*, (03 2011): 1765. doi:
- 12/19/2012 27.00 A.Y. Borisevich, E.A. Eliseev, A.N. Morozovska, C.-J. Cheng, J.-Y. Lin, Y.H. Chu, D. Kan, I. Takeuchi, V. Nagarajan, S.V. Kalinin<sup>1</sup>. Atomic-scale evolution of modulated phases at the ferroelectric–antiferroelectric morphotropic phase boundary controlled by flexoelectric interaction, *Nature Communications*, (04 2012): 1. doi:
- 12/19/2012 26.00 Tiberiu-Dan Onuta, Yi Wang, Christian J. Long, Samuel E. Lofland, Ichiro Takeuchi. Dynamic state switching in nonlinear multiferroic cantilevers, *Applied Physics Letters* (accepted), (07 2012): 43506. doi:
- 12/19/2012 25.00 Yiming Wu, Jan Muehlbauer, Yunho Hwang, Reinhard Radermacher, Jun Cui, Sean Fackler, Manfred Wuttig, Ichiro Takeuchi. Demonstration of high efficiency elastocaloric cooling with large DT using NiTi wires, *Applied Physics Letters* (accepted), (08 2012): 73904. doi:
- 12/19/2012 33.00 Remi Delville, Hui Shi, Richard D. James, Dominique Schryvers. Special microstructures and twin features in Ti<sub>50</sub>Ni<sub>50-x</sub>(Pd,Au)<sub>x</sub> at small hysteresis, *Solid State Phenomena*, (06 2011): 105. doi:
- 12/19/2012 34.00 Vijay Srivastava, Yintao Song, Kanwal Bhatti, R. D. James. The direct conversion of heat to electricity using multiferroic alloys, *Advanced Energy Materials*, (01 2011): 97. doi:
- 12/19/2012 35.00 J. K. Kawasaki, J. Buschbeck, A. Kozhanov, R. D. James, C. J. Palmstrøm. Martensite transformations in epitaxial Ni-Ti shape memory alloy films, *Applied Physics Letters*, (05 2011): 191901. doi:
- 12/19/2012 22.00 Gregory S. Pomrehn, Eric S. Toberer, G. Jeffrey Snyder, Axel van de Walle. Predicted Electronic and Thermodynamic Properties of a Newly Discovered Zn<sub>8</sub>Sb<sub>7</sub> Phase, *Journal of the American Chemical Society*, (06 2011): 11255. doi:
- 12/19/2012 23.00 Gregory S. Pomrehn, Eric S. Toberer, G. Jeffrey Snyder, Axel van de Walle. Entropic stabilization and retrograde solubility in Zn<sub>4</sub>Sb<sub>3</sub>, *Physics Rev. B*, (03 2011): 94106. doi:
- 12/20/2012 24.00 P. H. Michael Böttger, Gregory S. Pomrehn, G. Jeffrey Snyder, Terje G. Finstad. Dynamic state switching in nonlinear multiferroic cantilevers, *Physica Status Solidi*, (12 2011): 2753. doi:
- 12/20/2012 40.00 Kaushik Bhattacharya, Phanish Suryanarayana, Michael Ortiz. Coarse-graining Kohn–Sham Density Functional Theory, *Journal of the Mechanics and Physics of Solids*, (09 2012): 38. doi:
- 12/20/2012 41.00 Hsin-Yi Kuo, Alex Slinger, Kaushik Bhattacharya. Optimization of magnetoelectricity in piezoelectric–magnetostriuctive bilayers, *Smart Materials and Structures*, (08 2010): 125010. doi:
- 12/20/2012 43.00 Phanish Suryanarayana, Kaushik Bhattacharya. Evolution of polarization and space charges in semiconducting ferroelectrics, *Journal of Applied Physics*, (02 2012): 34109. doi:
- 12/20/2012 44.00 Vivek B. Shenoy, Kaushik Bhattacharya. Effect of doping on polarization profiles and switching in semiconducting ferroelectric thin films, *Journal of Applied Physics*, (04 2012): 84105. doi:
- 12/20/2012 46.00 Teruyuki Ikeda<sup>a</sup>, Nathan J. Marolf<sup>b</sup>, Kristin Bergum<sup>b</sup>, Marcus B. Toussaint<sup>b</sup>, Nicholas A. Heinz<sup>b</sup>, Vilupanur A. Ravi<sup>c</sup>, G. Jeffrey Snyder. Size control of Sb<sub>2</sub>Te<sub>3</sub> Widmanstätten precipitates in thermoelectric PbTe, *Acta Materialia*, (04 2011): 2679. doi:

12/20/2012	45.00	Daisuke Kan, Wangchun Chen, Shannon Watson, Songxue Chi, Ross Erwin, Garry J. McIntyre, Sylvia C. Capelli, William Ratcliff , Ichiro Takeuchi.. Neutron Diffraction Investigations of Magnetism in BiFeO3 Epitaxial Films, Advanced Functional materials , (03 2011): 1567. doi:
12/20/2012	47.00	Kristin Berguma, Teruyuki Ikeda, G. Jeffrey Snyder. Solubility and microstructure in the pseudo-binary PbTe–Ag2Te system, Journal of Solid State Chemistry, (09 2011): 2543. doi:
12/20/2012	48.00	Teruyuki Ikeda, Shiho Iwanaga, Hsin-jay Wu, Nathan J. Marolf, Sinn-wen Chen, G. Jeffrey Snyder . A combinatorial approach to microstructure and thermopower of bulk thermoelectric , Journal of Materials Chemistry, (06 2012): 24335. doi:

**TOTAL: 121**

**Number of Papers published in peer-reviewed journals:**

**(b) Papers published in non-peer-reviewed journals (N/A for none)**

<u>Received</u>	<u>Paper</u>
09/03/2013	28.00 Richard D. James, Vivekanand Dabade, Xian Chen, Vijay Srivastava. Study of the cofactor conditions: conditions of supercompatibility between phases , Journal of the Mechanics and Physics of Solids, (08 2013): 0. doi:
12/18/2012	15.00 Teruyuki Ikeda, Shiho Iwanaga, Hsin-jay Wu, Nathan J. Marolf, Sinn-wen Chen, G. Jeffrey Snyder . A combinatorial approach to microstructure and thermopower of bulk thermoelectric , Journal of Materials Chemistry, (06 2012): 24335. doi:
12/18/2012	16.00 Kristin Berguma, Teruyuki Ikeda, G. Jeffrey Snyder. Solubility and microstructure in the pseudo-binary PbTe–Ag2Te system, Journal of Solid State Chemistry, (09 2011): 2543. doi:
12/18/2012	17.00 Teruyuki Ikeda, Nathan J. Marolf, Kristin Bergum, Marcus B. Toussaint, Nicholas A. Heinz, Vilupanur A. Ravic, G. Jeffrey Snyder. Size control of Sb2Te3 Widmanstätten precipitates in thermoelectric PbTe, Acta Materialia, (04 2011): 2679. doi:
12/19/2012	31.00 Daisuke Kan, Wangchun Chen, Shannon Watson, Songxue Chi, Ross Erwin, Garry J. McIntyre, Sylvia C. Capelli, William Ratcliff II, Ichiro Takeuchi. Neutron Diffraction Investigations of Magnetism in BiFeO3 Epitaxial Films , Advanced Functional Materials, (03 2011): 1567. doi:

**TOTAL: 5**

**Number of Papers published in non peer-reviewed journals:**

**(c) Presentations**

Kaushik Bhattacharya:

International Congress of Theoretical and Applied Mechanics, Beijing, Aug. 2012 (Sectional Lecture).

PIRE Summer School on New Frontiers in Multiscale Analysis and Computing for Materials, Minneapolis Jun. 2012 (Six Lectures).

Sossina Haile:

"Phase Behavior of Superprotonic Solid Acid Electrolytes," Plenary Lecture, 16th International Conference on Solid State Proton Conductors, Sept 9-13, 2012, Grenoble, France

"Phase Behavior of Proton-conducting Oxyanion Solid Acid Electrolytes," Keynote Lecture, 19th International Conference on Solid State Ionics, May 2-7, 2013, Kyoto, Japan

Ichiro Takeuchi:

"Thermoelastic cooling and multiferroic devices," Multifunctional Materials Workshop, Panama, August 8th

"Combinatorial approaches to multifunctional materials," Dept seminar, MSE, NCSU, August 31st

"Multiferroic devices," Dept seminar, Electrical Engineering, Northeastern Univ., September 20th

"Data-driven approaches to combinatorial materials discovery," Materials Genome Initiative Workshop, October 4th

"Combinatorial search for rare-earth free permanent magnets," Int. Workshop on Combinatorial Materials Science, Charleston, South Carolina, October 23rd

"Thermoelastic cooling," UK Royal Society Seminar, London, UK, February 19th, 2013

"Data-driven approaches to combinatorial strategy," DPG Meeting, Regensburg, Germany, March 12, 2013

"Combinatorial discovery of lead-free piezoelectric materials," Piezoelectric Materials Workshop, April 9th

"Combinatorial search of multifunctional materials," Nano Electronic Materials Symposium, Kanazawa, Japan, June 19th

"Thermoelastic cooling," Univ. of Tokyo Seminar Day, Kashiwa, Japan, June 26th

"Thermoelastic cooling," Banff Research Station, Banff, Canada, July 18th

Jeff Snyder:

December 2012 "Thermoelectrics Materials for Energy" JUAMI workshop, Addis Abeba, Ethiopia.

November 2012 "Band Structure Engineering of Thermoelectric Materials" Wuhan, China

September 2012 "Complex Thermoelectric Materials" U. Tokyo, Japan

September 2012 "The Thomson cooler derived from the Compatibility Factor Approach to the analysis of Thermoelectric Devices" Workshop on Thermoelectrics, Waseda University, Japan

September 2012 "Complex Thermoelectric Materials" Shizuoka U., Japan

September 2012 "Band Engineering for High Efficiency Thermoelectrics" IUMRS, Yokohama, Japan

July 2012 "Designing Thermoelectric Transport in Zintl Phases" Solid State Chemistry Gordon Conference, NH

June 2012 "Band Engineering for Thermoelectrics" Martin Luther University, Halle, Germany

June 2012 "Complex Thermoelectric Materials" Nature Conference, Aachen Germany

March 2012 "Optimizing overall Efficiency in Thermoelectric Generators" DOE-Thermoelectric Applications Workshop, Baltimore MD.

February 2012 "Complex Thermoelectric Materials" Visiting Professor Lecture, Wuhan Institute of Technology, Wuhan China.

January 2012 "Band Engineering for Thermoelectrics" Indo-USA workshop, Mumbai, India

Jiangyu Li

-Nanoscale Electromechanics in Biology, 7th International Conference on Materials for Advanced Technology, Nanoscale Electromechanics in Biology, Singapore, July 2013.

-Nanoscale Electromechanics: from Biological Ferroelectricity to Li-ion Batteries, IUTAM Symposium on Hysteresis and Pattern Evolution in Non-equilibrium Solid-Solid Phase Transitions, Hong Kong, China, August, 2012.

Richard James

-2012 James K. Knowles Lecture, Caltech (\$3^{\rm rd}\$ in this series), ``Materials for the direct conversion of heat to electricity"

-Keynote Lecture (one of three), ASME Conference on Smart Materials, Adaptive Structures and Intelligent Systems, Stone Mountain, GA,  
``The direct conversion of heat to electricity using multiferroic materials with phase transformations"

-2013 Pedro Nunes Lectures, Lisbon, ``New methods for the direct conversion of heat to electricity suggested by geometry"; also, an  
advanced course on ``Compatibility, hysteresis and the direct conversion of heat to electricity" (Lisbon)

-Lecture series on ``Compatibility, hysteresis and energy conversion,  
CNA Summer School, Carnegie Mellon (5 lectures, May 30 - June 7 )

-Plenary Lecture, Mandel Symposium, ``Compatibility, hysteresis and the direct conversion of heat to electricity" (June 27)

-Colloquia at Rutgers, UW Seattle,

**Number of Presentations:** 35.00

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**Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**

<u>Received</u>	<u>Paper</u>
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**TOTAL:**

**Number of Non Peer-Reviewed Conference Proceeding publications (other than abstracts):**

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**Peer-Reviewed Conference Proceeding publications (other than abstracts):**

<u>Received</u>	<u>Paper</u>
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**TOTAL:**

**Number of Peer-Reviewed Conference Proceeding publications (other than abstracts):**

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**(d) Manuscripts**

Received                      Paper

08/30/2013	18.00	D. Kitchaev , S. M. Haile, A. Ikeda. Phase behavior and superprotonic conductivity in the Cs1-xRbxH2PO4 and Cs1-xKxH2PO4 systems” , Chemistry of Materials ( )
12/20/2012	42.00	Hsin-Yi Kuo, Kaushik Bhattacharya□. Fibrous composites of piezoelectric and piezomagneticphases, Mechanics of Materials (06 2012)

**TOTAL:                      2**

**Number of Manuscripts:**

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**Books**

Received                      Paper

**TOTAL:**

**Patents Submitted**

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**Patents Awarded**

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**Awards**

Kaushik Bhattacharya:

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Fellow, Society for Industrial and Applied Mathematics, 2013.

Graduate Student Council Teaching and Mentoring Award, California Institute of Technology, 2013.

Jiangyu Li

-Jiangyu Li was promoted to Full Professor at the University of Washington in 2013.

Ichiro Takeuchi:

-A continuation of an earlier project, which was partially supported by the MURI, on thermoelastic cooling was funded by ARPA-E.

-The above invited review appeared on the cover of Journal of Applied Physics (attached)

-We started a new collaboration on combinatorial investigation of materials for solid oxide fuel cells with Sossina Haile.

Jeff Snyder:

Jeff Snyder, Elected Treasurer of the Board of Directors of the International Thermoelectric Society

Yanzhong Pei (Postdoc of Snyder) received the Young Investigator Award for outstanding postdoctoral work in thermoelectrics at International Conference in Thermoelectrics, Kobe Japan, June 2013.

Alex Zevalkink (Student of Snyder) received the Goldsmid Award for outstanding graduate work in thermoelectrics at International Conference in Thermoelectrics, Kobe Japan, June 2013.

Eric Toberer (Postdoc of Snyder) received the Young Investigator Award for outstanding postdoctoral work in thermoelectrics at International Conference in Thermoelectrics, Traverse city, June 2011.

Andrew May (Student of Snyder) received the Goldsmid Award for outstanding graduate work in thermoelectrics at International Conference in Thermoelectrics, Shanghai China, May 2010.

Andrew May (Student of Snyder) received the Demetriades-Tsafka-Kokkalis Prize for outstanding graduate work in sustainable energy at Caltech, June 2010.

Jiangyu Li, 2008 ICCES Young Investigator Award in Theory; 2008 Nemat-Nasser Early Career Medal, American Society of Mechanical Engineers; Engineers; MURI supported research chosen as PRL editors' suggestion, featured by BBC, New Scientist, Inside Science News Service, APS Physics Viewpoint, and highlighted by Nature Nanotechnology, NSF News, and many other media.

Karen Rabe, 2008 David Adler Lecturership Award of the American Physical Society

Sossina Haile, 2008 NSF American Competitiveness Initiative (ACI) Fellow; 2008 Lucy Pickett Lecturer in Chemistry at Mount Holyoke College; 2009 Dow Distinguished Lecturer at UCSB; 2010 Chemical Pioneer Award of the American Institute of Chemists; 2010 Outstanding Women in Science Lecturer, University of Indiana, Bloomington; International Ceramics Prize (World Academy of Ceramics) 2012; Carl Braun Professorship, 2012.

Kaushik Bhattacharya, 2007-2008 Southwest Mechanics Lecturer, Howell N. Tyson Professor of Mechanics.

Ichiro Takeuchi, 2008 invited participant of the US Frontiers of Engineering Symposium of the National Academy of Engineering

Richard James, 2008 Prager Medal of the Society of Engineering Science; 2008 Drucker Medal of American Society of Mechanical Engineers; 2009 Brown Engineering Alumni Medal

Jeff Snyder, Elected to the Board of Directors of the International Thermoelectric Society

Mary Louie, (student of Haile) Dokiya Fund (in support of attendance of SSPC 14, Sept 7-11, 2008, Kyoto, Japan), - ECS Student Travel Grant (from the Energy Technology Division), in support of attendance at the 213th Meeting of the Electrochemical Society, May 18-23, 2008, Phoenix, AZ; 2008 Ludo Frevel Crystallography Scholarship Award; 2008 Baker Hughes Scholarship of the Society of Women Engineers

Chris Long (student of Takeuchi), 2009 Ludo Frevel Crystallography Scholarship Award

Chris Palmstrøm, 2012 MRS Fellow; 2008, 2011 Elected secretary/treasurer of APS Division of Materials Physics

Jason Kawasaki (student of Palmstrøm), 2012 MRS Student Gold Award, 2011 North American MBE student award

Ichiro Takeuchi was elected fellow of American Physical Society 2010

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**Graduate Students**

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	Discipline
Yi Wang	0.00	
Ayako Ikeda	0.00	
Chatr Panithipongwut	0.00	
Greg Pomrhen	0.00	
Nick Heinz	0.00	
Yuanming Liu	0.00	
Xian Chen	0.00	
Yintao Song	0.00	
Bharat P. Penmecha	0.00	
<b>FTE Equivalent:</b>	<b>0.00</b>	
<b>Total Number:</b>	<b>9</b>	

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**Names of Post Doctorates**

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
Tiberiu Onuta	0.00
Teruyuki Ikeda	0.00
Eric Toberer	0.00
Vijay Srivastava	0.00
Kanwal Bhatti	0.00
<b>FTE Equivalent:</b>	<b>0.00</b>
<b>Total Number:</b>	<b>5</b>

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**Names of Faculty Supported**

<u>NAME</u>	<u>PERCENT SUPPORTED</u>	National Academy Member
Richard D. James	1.00	
Ichio Takeuchi	1.00	
Jiangyu Li	1.00	
Sossina Haile	1.00	
Jeff Snyder	1.00	
Chris Palmstrom	1.00	
Harry Atwater	1.00	
Kaushik Bhattacharya	1.00	
Karin Rabe	1.00	
Manfred Wuttig	1.00	
<b>FTE Equivalent:</b>	<b>10.00</b>	
<b>Total Number:</b>	<b>10</b>	

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**Names of Under Graduate students supported**

<u>NAME</u>	<u>PERCENT SUPPORTED</u>
<b>FTE Equivalent:</b>	
<b>Total Number:</b>	



### Student Metrics

This section only applies to graduating undergraduates supported by this agreement in this reporting period

The number of undergraduates funded by this agreement who graduated during this period: ..... 0.00

The number of undergraduates funded by this agreement who graduated during this period with a degree in science, mathematics, engineering, or technology fields:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will continue to pursue a graduate or Ph.D. degree in science, mathematics, engineering, or technology fields:..... 0.00

Number of graduating undergraduates who achieved a 3.5 GPA to 4.0 (4.0 max scale): ..... 0.00

Number of graduating undergraduates funded by a DoD funded Center of Excellence grant for Education, Research and Engineering:..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and intend to work for the Department of Defense ..... 0.00

The number of undergraduates funded by your agreement who graduated during this period and will receive scholarships or fellowships for further studies in science, mathematics, engineering or technology fields: ..... 0.00

### Names of Personnel receiving masters degrees

NAME

**Total Number:**

### Names of personnel receiving PhDs

NAME

Xian Chen

Yintao Song

Bharat P. Penmecha

**Total Number:**

3

### Names of other research staff

NAME

Leslie Rico

**FTE Equivalent:**

**Total Number:**

PERCENT SUPPORTED

0.00

**0.00**

1

### Sub Contractors (DD882)

### Inventions (DD882)

## Scientific Progress

The MURI project has opened a new path towards unprecedented multifunctional materials. The research in the project has unequivocally established that it is possible to have first order structural transformation with virtually no hysteresis and with little limitation on the extent of structural change. Since electronic structure and consequently electrical, magnetic, optical and mechanical properties depend on structure, structural phase transformation provides a way of coupling an unusual combination of electrical, magnetic, optical and mechanical properties. The project has discovered new materials, developed new experimental and theoretical tools and demonstrated prototype applications.

A few highlights of the results of the MURI project.

- Discovery of a new lead-free piezoelectric material. Takeuchi et al. have demonstrated that (Bi,Sm) FeO<sub>3</sub> has a morphotropic phase boundary at about 14 at% Sm. The piezoelectric coefficient  $d_{33}$  is 110 pm/V and the dielectric coefficient  $\epsilon_{33}$  is over 400 while loss factor ( $\tan \delta$ ) remains low at less than 0.02 at this composition. These are comparable to the commercial PZT. This material was discovered through a combinatorial search. Rabe et al. have used first principles methods to show that this morphotropic boundary happens as a result of an electrically-driven phase transition. Bhattacharya and Li have suggested that hysteresis is low because of frustration at this composition.
- Discovery of a suite of new low-hysteresis shape-memory alloys. James, Takeuchi, Wuttig et al. have developed a very large number of shape-memory alloys with extremely low hysteresis. These are tertiary and quaternary modifications of NiTi and the best alloys have a thermal hysteresis lower than 1K with significant transformation strain. These alloys were developed using a strategy suggested by James based on theoretical analysis that materials with compatible interfaces – mathematically where the middle eigenvalue of the transformation matrix is one – would display very little hysteresis. James et al. have also shown that these alloys display a habit plane with no internal twinning.
- Discovery of a low-hysteresis Heusler alloy with unusual magnetic properties. James, Wuttig et al. have shown that Ni<sub>45</sub>Co<sub>5</sub>Mn<sub>40</sub>Sn<sub>10</sub> undergoes a martensitic transformation with significant strain and very little hysteresis. Further, this alloy becomes magnetized with a magnetization of about 100 emu/cc at the transformation temperature. James et al. have suggested a new strategy for energy recovery from waste heat using this alloy.
- Discovery of a new fatigue-free shape-memory alloy and a thermoelectric air-conditioner. James, Takeuchi et al. have shown that the low hysteresis shape-memory alloys also have extremely long fatigue life. Takeuchi et al. have used this material to a prototype a 1kW thermoelectric air-conditioner using this alloy.
- A new strategy for the phase-transforming thin films. While phase transformations enable various functional properties, it is difficult to implement these in thin films where the substrate constrains these transformations. Palmström, James et al. have explored a new strategy where the orientation of the film is epitaxially chosen to be coincident to the twin-free habit plane. This enables large shape-change during transformation with no interference from the substrate.
- Three strategies to obtaining hysteresis-free materials. The MURI team proposed and exploited three different strategies to obtain materials that undergo first order phase transitions with very little hysteresis. (i) James suggested based on a theoretical analysis that compatible interfaces – mathematically where the middle eigenvalue of the transformation matrix is one – would display very little hysteresis. The MURI team has demonstrated this in a number of material systems. (ii) Bhattacharya and Li showed that frustration can give rise to the morphotropic phase boundaries in perovskite systems, and that the hysteresis would be small at these morphotropic phase boundaries. Wuttig et al. used a novel diblock copolymer based sol-gel synthesis to create a microstructure of triangular array of ferromagnetic columns in a piezoelectric matrix. The antiferromagnetic coupling between the columns gave rise to frustration and this led to electro-magnetic coupling with very small hysteresis. (iii) Wuttig, Takeuchi et al. have recently shown that nanoscale defects in magnetic materials with a long exchange length can give rise to extremely low hysteresis.
- Exploitation of electronic structure calculations to predict new and unusual phase transitions. Rabe has developed a strategy to use first principle calculations to identify potential phase transitions. The strategy is to use phonon dispersion to identify soft modes, and then stabilize them using external fields like electric field, chemical pressure or epitaxial strain. This strategy identified the source of the morphotropic boundary in (Bi,Sm) Fe O<sub>3</sub>.
- New theoretical and experimental methods. The MURI developed a host of new theoretical and experimental methods. These include a new method for studying extended crystal defects using density functional theory (Bhattacharya), a new method of identifying transformation strains based on x-ray diffraction data (James), a new scanning probe approach to studying electromechanical coupling (Li), an environmental chamber to conduct x-ray diffraction at controlled humidity (Haile) and a new high-throughput approach to x-ray diffraction (Takeuchi).
- Novel applications of multifunctional materials. Atwater et al. have developed a number of tunable photonic devices where strain is used to tune the device characteristics. Current research seeks to integrate it with Au-Cu-Zn shape-memory alloy. James et al. have suggested a new strategy for energy recovery from waste heat using low-hysteresis based Heusler alloys. Takeuchi et al. have used the high fatigue life shape-memory alloy to prototype a 1kW thermoelectric air-conditioner using this alloy.
- To date the project has contributed to the training of over 30 graduate students and 10 post-doctoral scholars, and resulted in over 100 peer-reviewed journal publications, over 70 conference talks (including plenary talks) and 3 patents.

## Technology Transfer